Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
S23	95	(568/902).CCLS.	US-PGPUB; USPAT	OR	OFF	2004/04/15 16:02
S24	95	568/902.ccls.	US-PGPUB; USPAT	OR	OFF	2004/04/15 16:28
S25	11	S24 and (propanediol or 3-propanediol or diol)	US-PGPUB; USPAT	OR	OFF	2004/04/15 16:03
S26	328	568/678	US-PGPUB; USPAT	OR	OFF	2004/04/15 16:31
S27	23	568/678.ccls. and propanediol	US-PGPUB; USPAT	OR	OFF	2004/04/15 16:31

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     FILE 'BEILSTEIN' ENTERED AT 17:53:37 ON 15 APR 2004
L3               STRUCTURE UPLOADED
L4          617733 S 2/O  NOT N/ELS
L5          526528 S L4 NOT (S/ELS OR X/ELS OR M/ELS)
L6          526528 S L5 NOT PMS/CI
L7              46 S L3  SUB=L5 FULL
L8               0 S L7 AND 1-5/NR
L9               8 S L7 AND PHENY?
L10             38 S L7 NOT L9
L11              2 S L10 AND (ISOPRO? OR METHYLETHYL OR TERTIARY BUTYL )

=> s l10 not l11
L12             36 L10 NOT L11

=> s l12 and penty?
          97437 PENTY?
L13              0 L12 AND PENTY?

=> d ide l12 30


L12  ANSWER 30 OF 36 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

      Beilstein Records (BRN):          1851103
      Beilstein Pref. RN (BPR):         60851-88-9
      CAS Reg. No. (RN):                60851-88-9
      Chemical Name (CN):               3-decyloxy-propan-1-ol
      Autonom Name (AUN):               3-decyloxy-propan-1-ol
      Molec. Formula (MF):              C13 H28 O2
      Molecular Weight (MW):            216.36
      Lawson Number (LN):               523, 362
      Compound Type (CTYPE):            acyclic
      Constitution ID (CONSID):         1696104
      Tautomer ID (TAUTID):             1757099
      Beilstein Citation (BSO):         5-01, 6-01
      Entry Date (DED):                 1989/06/29
      Update Date (DUPD):               2003/10/23
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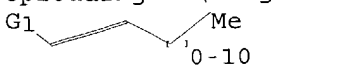
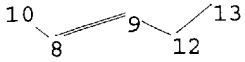
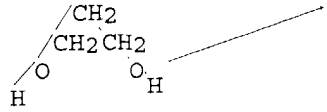
Field Availability:

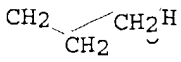
Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	2
ED	Entry Date	1

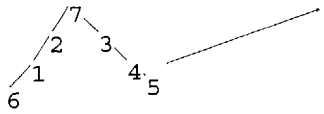
=>
Uploading C:\Program Files\Stnexp\Queries\10679174.str

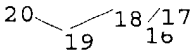












chain nodes :
1 2 3 4 5 6 7 8 9 10 12 13 16 17 18 19 20
chain bonds :
1-2 1-6 2-7 3-4 3-7 4-5 8-9 8-10 9-12 12-13 16-17 16-18 18-19 19-20

exact/norm bonds :
8-10
exact bonds :
1-2 1-6 2-7 3-4 3-7 4-5 8-9 9-12 12-13 16-17 16-18 18-19 19-20

G1:H,Ak,Cb

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 12:CLASS 13:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
fragments assigned product role:
containing 16
fragments assigned reactant/reagent role:
containing 1
containing 8

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 13:47:04 FILE 'CASREACT'
SCREENING COMPLETE - 4638 REACTIONS TO VERIFY FROM 446 DOCUMENTS

100.0% DONE 4638 VERIFIED 0 HIT RXNS 0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**

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PROJECTED VERIFICATIONS:      88699 TO     96821
PROJECTED ANSWERS:                0 TO         0

L2             0 SEA SSS SAM L1 (      0 REACTIONS)

=> s l1 full
FULL SEARCH INITIATED 13:47:11 FILE 'CASREACT'
SCREENING COMPLETE -  98286 REACTIONS TO VERIFY FROM   9143 DOCUMENTS

100.0% DONE  98286 VERIFIED      11 HIT RXNS                      6 DOCS
SEARCH TIME: 00.00.12

L3             6 SEA SSS FUL L1 (     11 REACTIONS)

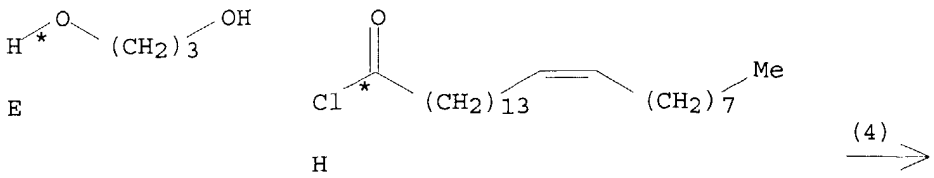
=> d ibib abs fhit 1-6


L3   ANSWER 1 OF 6  CASREACT  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         135:14317  CASREACT
TITLE:                    Nervonic acid derivatives, their preparation, and
                          anti-inflammatory and immunomodulatory use
INVENTOR(S):              Coupland, Keith; Raoul, Yann
PATENT ASSIGNEE(S):       Croda International PLC, UK
SOURCE:                   PCT Int. Appl., 54 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

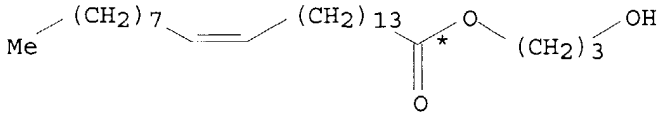
     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ----------------  ----  --------       ---------------  --------
     WO 2001038288      A1   20010531       WO 2000-GB4453   20001123
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     GB 2357083         A1   20010613       GB 2000-28525    20001123
     GB 2357083         B2   20020619
     EP 1232139         A1   20020821       EP 2000-977695   20001123
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     JP 2003514886      T2   20030422       JP 2001-539845   20001123
     NZ 518961          A    20040227       NZ 2000-518961   20001123
     US 6664406         B1   20031216       US 2002-130672   20020819
PRIORITY APPLN. INFO.:                       GB 1999-27629    19991124
                                             WO 2000-GB4453   20001123

OTHER SOURCE(S):          MARPAT 135:14317
AB   The invention discloses nervonic acid derivs.
     CH3(CH2)7CH:CH(CH2)13C(O)O(CH2)3OR (R = H, carboxylic acid residue), or a
     salt of the compound where R is H, or a bioprecursor, prodrug or hydrate
     thereof.  Those compds. wherein R is other than H have pharmacol.
     activity, in particular anti-inflammatory and immunomodulatory effects.
     Those compds. wherein R is H can be used to prepare the pharmacol. active
     derivs.


RX(4) OF 14      ...E  +  H  ===>  A...
```



E H (4)



A

RX(4) RCT E **504-63-2**

STAGE(1)
RGT K 121-44-8 Et3N
SOL 75-09-2 CH2Cl2

STAGE(2)
RCT H **145411-43-4**
SOL 75-09-2 CH2Cl2
PRO A **342573-48-2**

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 6 CASREACT COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 114:42757 CASREACT
TITLE: Synthesis of methyl-substituted lariat ethers containing a 13-crown-4 ring
AUTHOR(S): Wakita, Ryuhei; Yonetani, Masayuki; Nakatsuji, Yohji; Okahara, Mitsuo
CORPORATE SOURCE: Fac. Eng., Osaka Univ., Osaka, 565, Japan
SOURCE: Journal of Heterocyclic Chemistry (1990), 27(5), 1337-9
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
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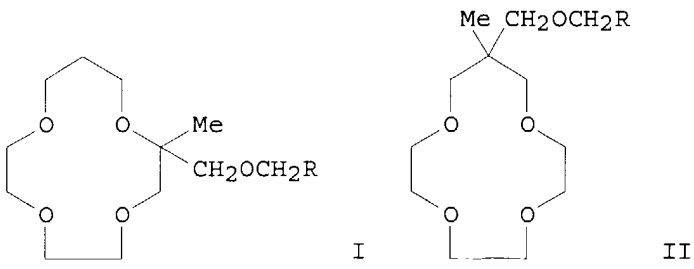
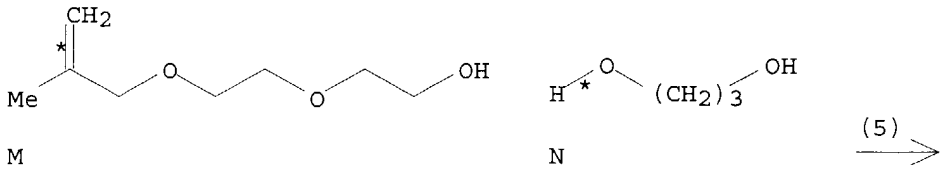


I II

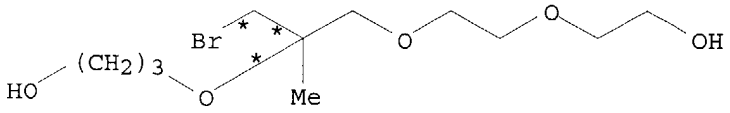
AB Convenient synthetic procedures for preparing two kinds of methyl-substituted

lariat ethers containing a 13-crown-4-ring, I and II [R = CH2OMe, (CH2)8Me, 2-tetrahydrofuryl], are described. I were obtained from the reaction of 2-bromomethyl-2-methyl-13-crown-4 (III) with the appropriate alkoxide. III was prepared without the need for prior protection of the bromomethyl group. For the synthesis of II, which possess an electron-donating group on the central carbon of the tri-Me moiety of the 13-crown-4-ring, the substituents were introduced before cyclization.

RX(5) OF 9 **M** + **N** ===> **I**...



M N



I
YIELD 48%

RX(5) RCT M **121343-32-6**, N **504-63-2**
RGT L 128-08-5 Bromosuccinimide
PRO I **131526-53-9**
SOL 504-63-2 HO(CH2)3OH

L3 ANSWER 3 OF 6 CASREACT COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 109:73744 CASREACT
TITLE: Stereoselective synthesis of 25-hydroxyvitamin D2 side chain via the acetal template route
AUTHOR(S): Castedo, L.; Granja, J.; Maestro, M. A.; Mourino, A.
CORPORATE SOURCE: Dep. Quim. Org., Fac. Quim., Santiago de Compostela, Spain
SOURCE: Tetrahedron Letters (1987), 28(39), 4589-90
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
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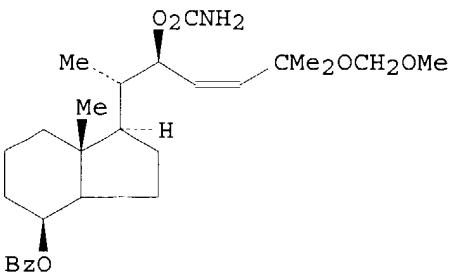
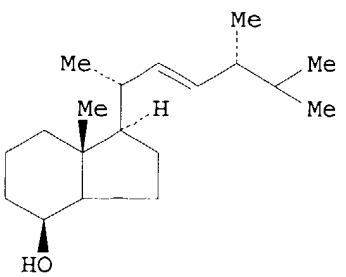


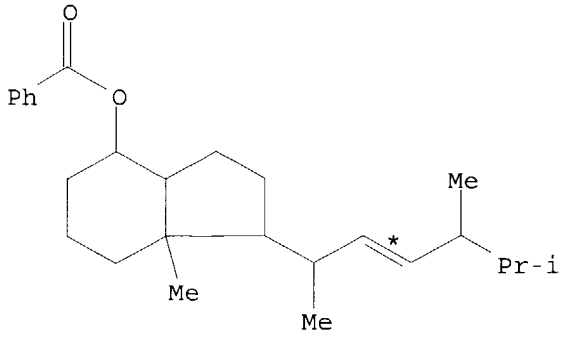
I



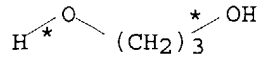
II

AB An improved synthesis of the vitamin intermediate I from II was described.

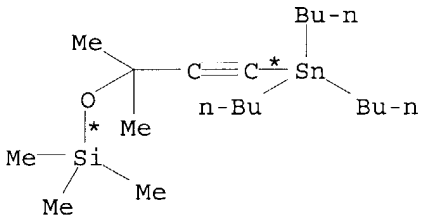
RX(31) OF 54 COMPOSED OF RX(2), RX(4), RX(8)
RX(31) 2 **C** + 2 **N** + 2 V ===> **W** + X



2 C

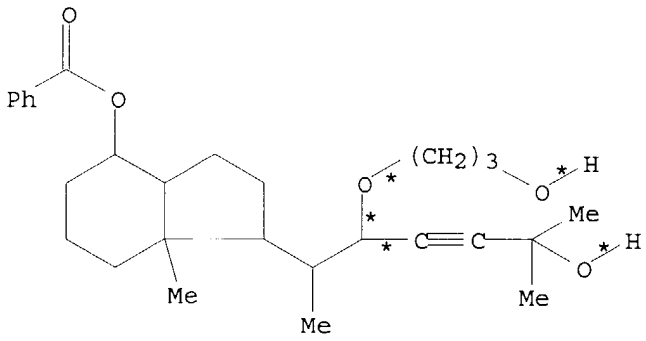


2 N

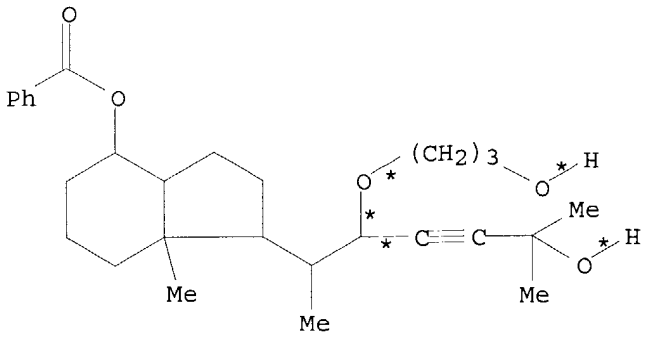


2 V

3
STEPS



W
YIELD 85%(67)



X
YIELD 85%(33)

RX(2) RCT C **68702-86-3**

STAGE(1)
RGT G 10028-15-6 Ozone, D 110-86-1 Pyridine
SOL 67-56-1 MeOH, 75-09-2 CH2Cl2

STAGE(2)
RGT H 122-52-1 P(OEt)3
SOL 67-56-1 MeOH, 75-09-2 CH2Cl2
PRO F 66774-71-8

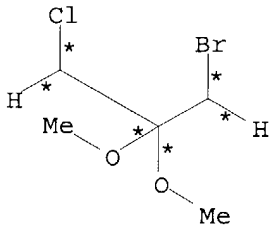
RX(4) RCT N **504-63-2**, F 66774-71-8
RGT P 109-63-7 BF3-Et2O
PRO O 115527-13-4
SOL 109-99-9 THF

RX(8) RCT V 115527-16-7, O 115527-13-4
RGT Y 7550-45-0 TiCl4
PRO W **115527-17-8**, X 115589-94-1
SOL 75-09-2 CH2Cl2

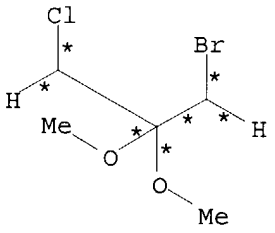
L3 ANSWER 4 OF 6 CASREACT COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 107:133679 CASREACT
TITLE: Thermal reactions of cyclopropenone ketals. Key mechanistic features and scope of the cycloaddition reactions of delocalized singlet vinylcarbenes: three-carbon 1,1-/1,3-dipoles
AUTHOR(S): Boger, Dale L.; Brotherton, Christine E.
CORPORATE SOURCE: Dep. Med. Chem., Univ. Kansas, Lawrence, KS, 66045-2500, USA
SOURCE: Journal of the American Chemical Society (1986), 108(21), 6695-713
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Full details of the key mechanistic features and the preparative scope of the thermal reactions of cyclopropenone ketals which proceed by the thermal generation and subsequent cycloaddn. reactions of π-delocalized singlet vinylcarbenes, 3-carbon 1,1-/1,3-dipoles lacking octet stabilization, are described and include ω2a participation in cheletropic [π2s + ω2a] nonlinear cycloaddns. with an observable endo effect suitable for a one-step, stereoselective construction of cis-cyclopropaneacetic acid esters, formal π2a participation in [π2s + π2a] cycloaddns. suitable for the preparation of functionalized

cyclopentenes in which each of the 5 carbons of the newly formed 5-membered ring may bear functionality capable of addnl. transformation, and π2a participation in [π4s + π2s] cycloaddns. with selected dienes in direct [3 + 4] cycloaddns. suitable for the preparation of functionalized cycloheptadienes capable of further elaboration to tropones/tropolones. The complementary scope of the thermal reactions of cyclopropenone ketals is demonstrated with the preparation of the complete range of (methoxycarbonyl)tropones, 2-, 3-, and 4-(methoxycarbonyl)tropone and tropone, utilizing the appropriate choice of starting diene and complementary choice of conditions for promoting the thermal [3 + 4] or [4 + 2] cycloaddn. of a cyclopropenone ketal. Addnl. details of a preliminary study of the scope of the cycloaddn. reactions of the apparent π-delocalized singlet vinylcarbene with C-heteroatom double bonds are described.

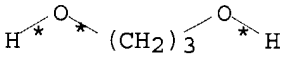
RX(91) OF 123 COMPOSED OF RX(51), RX(52), RX(6)
RX(91) 2 CO + 2 **CP** + 2 **N** ===> O + **M**



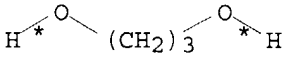
CO



CO



CP



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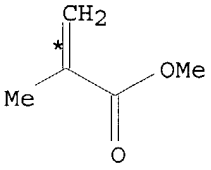
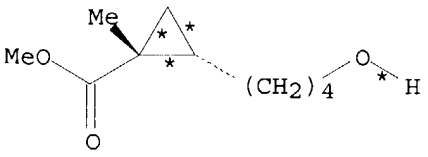
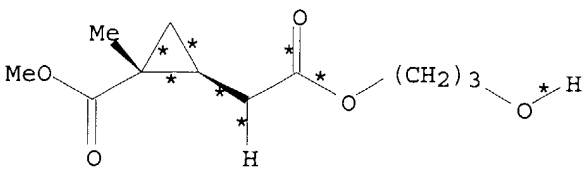


2 N

3
STEPS



O



M

RX(51) RCT CO 22089-54-9, CP **504-63-2**
RGT CM 7664-93-9 H2SO4
PRO CQ 60935-30-0
SOL 7732-18-5 Water

RX(52) RCT CQ 60935-30-0

RGT CR 17242-52-3 KNH2
PRO A 60935-21-9
CAT 7705-08-0 FeCl3
SOL 7664-41-7 NH3, 60-29-7 Et2O

RX(6) RCT A 60935-21-9, N 80-62-6
PRO O 103384-75-4, M **94923-06-5**
SOL 71-43-2 Benzene

L3 ANSWER 5 OF 6 CASREACT COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 106:213861 CASREACT
TITLE: Palladium(II)-catalyzed acetalization of terminal olefins bearing electron-withdrawing substituents with optically active diols
AUTHOR(S): Hosokawa, Takahiro; Ohta, Toshiyuki; Kanayama, Satoshi; Murahashi, Shunichi
CORPORATE SOURCE: Fac. Eng. Sci., Osaka Univ., Osaka, 560, Japan
SOURCE: Journal of Organic Chemistry (1987), 52(9), 1758-64
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
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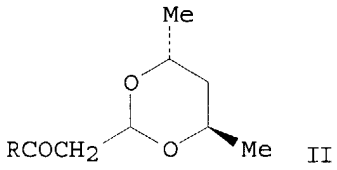
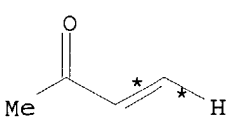


II

AB Terminal alkenes bearing electron-withdrawing substituents, such as CH2:CH2:CHCOR (R = Ph, Me, Me3C), CH2:CHCO2Me, and CH2:CHCN, are regioselectively acetalized at the terminal carbon by diols in the presence of PdCl2 and CuCl in MeOCH2CH2OMe at 50° under an atmospheric of O. The use of optically active (R,R)-2,4-pentanediol (I) gives homochiral cyclic acetals of aldehyde precursors, for example, II (R = Ph, Me, Me3C), in good yields. The reactivity of alkenes appears to decrease in the order: CH2:CHPh > CH2:CHCO2Me > CH2:CHCOR. Acetalization of CH2:CHCOR is accompanied by the formation of Michael-type adducts such as RCOCH2CH2OCHMeCH2CH(OH)Me. Their formation can be prevented by the use of Na2HPO4 as an additive. Although in an early stage of the reaction of CD2:CHPh with I, a statistical D scrambling of the starting alkene occurs, no such scrambling is observed with CD2:CHCOPh. Addnl., the acetalization of CD2:CHCOPh with I results in 1,2 deuterium migration, together with 25% D loss. These results are explained by reaction pathways involving oxypalladation, Pd-H elimination, and subsequent ring closure giving enol ether. A catalytic cycle involving the oxygenation of Pd-H species with mol. oxygen is proposed.

RX(9) OF 36 2 **J** + 2 **P** ===> S + **T**...



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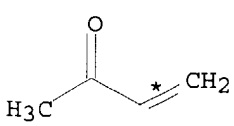

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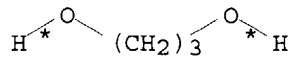
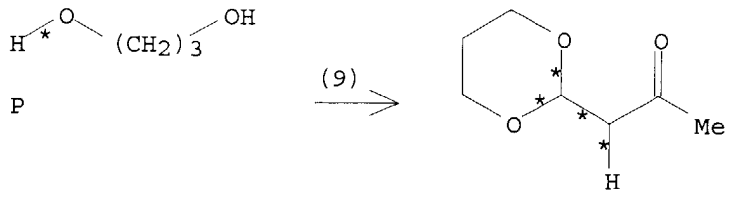
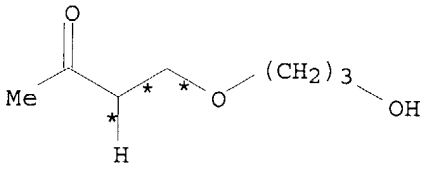


P



P

S
YIELD 45%

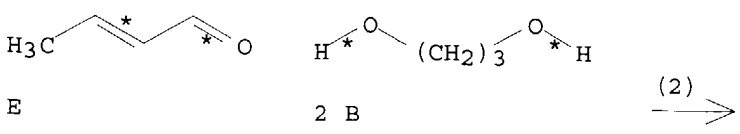


T
YIELD 8%

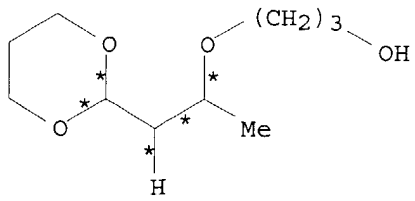
RX(9) RCT J **78-94-4**, P **504-63-2**
RGT E 7782-44-7 O2
PRO S 55558-31-1, T **87971-38-8**
CAT 7647-10-1 PdCl2, 7758-89-6 CuCl
SOL 110-71-4 (CH2OMe)2

L3 ANSWER 6 OF 6 CASREACT COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 102:220779 CASREACT
TITLE: Acetals and ethers - XIII. Reaction products of 2-butenal with ethylene glycol
AUTHOR(S): Piasecki, Andrzej
CORPORATE SOURCE: Inst. Org. Polym. Technol., Techn. Univ. Wroclaw, Wroclaw, 50-370, Pol.
SOURCE: Tetrahedron (1984), 40(23), 4893-6
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The unsatd. cyclic acetal, 2-(1-propenyl)-1,3-dioxolane, was an intermediate in the 4-MeC6H4SO3H-catalyzed reaction of 2-butenal with excess ethylene glycol. The final product was 2-[2-(2-hydroxyethoxy)propyl]-1,3-dioxolane, and a small amount of cis- and trans-5-(2-hydroxyethoxy)-7-methyl-1,4-dioxepane.

RX(2) OF 8 **E** + 2 **B** ===> **F**



E 2 B



F

RX(2) RCT E **4170-30-3**, B **504-63-2**
PRO F **96424-48-5**
CAT 104-15-4 TsOH

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	130.20	131.37

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-3.96	-3.96

FILE 'REGISTRY' ENTERED AT 13:48:19 ON 15 APR 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 14 APR 2004 HIGHEST RN 675571-70-7
DICTIONARY FILE UPDATES: 14 APR 2004 HIGHEST RN 675571-70-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

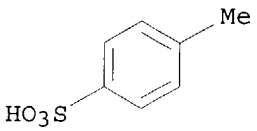
=> s tsoh
0 TSOH
L4 0 TSOH

=> s 104-15-4
L5 1 104-15-4
(104-15-4/RN)

=> d

L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN **104-15-4** REGISTRY
CN Benzenesulfonic acid, 4-methyl- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:
CN p-Toluenesulfonic acid (7CI, 8CI)
OTHER NAMES:
CN 4-Methylbenzenesulfonic acid
CN 4-Toluenesulfonic acid
CN Cyzac 4040
CN K-Cure 1040
CN Nacure 1040
CN NSC 167068
CN NSC 2167
CN p-Methylbenzenesulfonic acid
CN p-Methylphenylsulfonic acid
CN p-Toluenesulphonic acid
CN p-Tolylsulfonic acid
CN PTS 100
CN Toluenesulfonic acid
CN Tosic acid
AR 25231-46-3, 633305-48-3
FS 3D CONCORD
DR 402-47-1, 128739-80-0, 126033-27-0, 114213-96-6, 156627-46-2, 144647-92-7,
    100901-72-2, 210357-81-6, 227313-49-7, 369371-25-5, 613262-31-0
MF C7 H8 O3 S
CI COM
LC STN Files: AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS,
      BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS,
      CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, CSNB, DETHERM*, DIPPR*, EMBASE,
      ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*, HSDB*,
      IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC,
      PDLCOM*, PIRA, PROMT, PS, RTECS*, SPECINFO, TOXCENTER, TULSA, ULIDAT,
      USPAT2, USPATFULL
        (*File contains numerically searchable property data)
    Other Sources: DSL**, EINECS**, TSCA**
        (**Enter CHEMLIST File for up-to-date regulatory information)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

          9631 REFERENCES IN FILE CA (1907 TO DATE)
           356 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
          9644 REFERENCES IN FILE CAPLUS (1907 TO DATE)
             1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> d it 6 13
YOU HAVE REQUESTED DATA FROM FILE 'CASREACT' - CONTINUE? (Y)/N:y

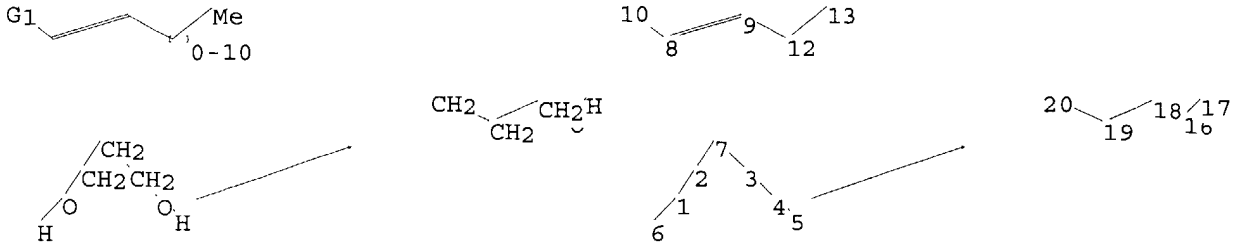
L3 ANSWER 6 OF 6 CASREACT COPYRIGHT 2004 ACS on STN
IT Acetals
    RL: RCT (Reactant); RACT (Reactant or reagent)
      (cyclic, of butenal)
IT 96424-45-2P 96424-46-3P 96424-50-9P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation and methylation or transacetalization of)

IT 96424-44-1P 96424-47-4P 96424-48-5P 96424-49-6P 96424-51-0P
96424-52-1P 96424-53-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 123-73-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethylene glycol or ethylene glycol monomethyl ether and trimethylene glycol)

=>
Uploading C:\Program Files\Stnexp\Queries\10679174.str



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chain bonds :
1-2 1-6 2-7 3-4 3-7 4-5 8-9 8-10 9-12 12-13 16-17 16-18 18-19 19-20

exact/norm bonds :
8-10
exact bonds :
1-2 1-6 2-7 3-4 3-7 4-5 8-9 9-12 12-13 16-17 16-18 18-19 19-20

G1:H,Ak,Cb

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 12:CLASS 13:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS
fragments assigned product role:
containing 16
fragments assigned reactant/reagent role:
containing 1
containing 8

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 15:22:07 FILE 'CASREACT'
SCREENING COMPLETE - 10610 REACTIONS TO VERIFY FROM 687 DOCUMENTS

47.1% DONE 5000 VERIFIED 0 HIT RXNS 0 DOCS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

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                          BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:    206105 TO   218295
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1 (     0 REACTIONS)

=> s l1 full
FULL SEARCH INITIATED 15:22:12 FILE 'CASREACT'
SCREENING COMPLETE - 202587 REACTIONS TO VERIFY FROM  13630 DOCUMENTS

100.0% DONE 202587 VERIFIED      24 HIT RXNS                     10 DOCS
SEARCH TIME: 00.00.17

L3           10 SEA SSS FUL L1 (    24 REACTIONS)

=> d his

     (FILE 'HOME' ENTERED AT 15:21:00 ON 15 APR 2004)

     FILE 'REGISTRY' ENTERED AT 15:21:15 ON 15 APR 2004

     FILE 'CASREACT' ENTERED AT 15:21:27 ON 15 APR 2004
L1               STRUCTURE UPLOADED
L2             0 S L1
L3            10 S L1 FULL

=> d ibib abs fhit 1-10


L3   ANSWER 1 OF 10  CASREACT  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         135:14317  CASREACT
TITLE:                    Nervonic acid derivatives, their preparation, and
                          anti-inflammatory and immunomodulatory use
INVENTOR(S):              Coupland, Keith; Raoul, Yann
PATENT ASSIGNEE(S):       Croda International PLC, UK
SOURCE:                   PCT Int. Appl., 54 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
     WO 2001038288      A1   20010531       WO 2000-GB4453   20001123
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     GB 2357083         A1   20010613       GB 2000-28525    20001123
     GB 2357083         B2   20020619
     EP 1232139         A1   20020821       EP 2000-977695   20001123
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     JP 2003514886      T2   20030422       JP 2001-539845   20001123
     NZ 518961          A    20040227       NZ 2000-518961   20001123
     US 6664406         B1   20031216       US 2002-130672   20020819
PRIORITY APPLN. INFO.:                      GB 1999-27629    19991124
                                            WO 2000-GB4453   20001123
```
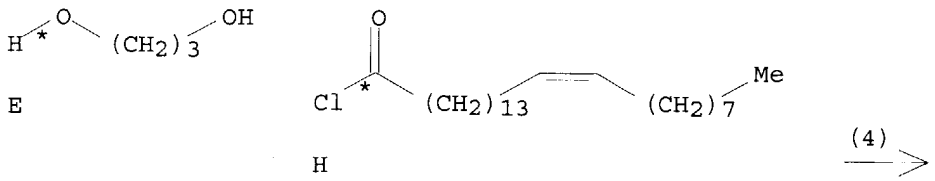

OTHER SOURCE(S): MARPAT 135:14317

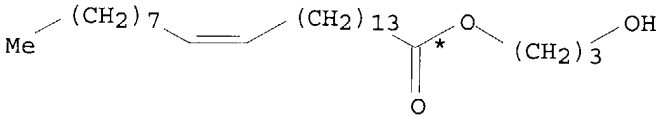
AB The invention discloses nervonic acid derivs. $CH_3(CH_2)_7CH{:}CH(CH_2)_{13}C(O)O(CH_2)_3OR$ (R = H, carboxylic acid residue), or a salt of the compound where R is H, or a bioprecursor, prodrug or hydrate thereof. Those compds. wherein R is other than H have pharmacol. activity, in particular anti-inflammatory and immunomodulatory effects. Those compds. wherein R is H can be used to prepare the pharmacol. active derivs.

RX(4) OF 14 ...**E** + **H** ===> **A**...



E H

(4)



A

RX(4) RCT E **504-63-2**

STAGE(1)
RGT K 121-44-8 Et3N
SOL 75-09-2 CH2Cl2

STAGE(2)
RCT H **145411-43-4**
SOL 75-09-2 CH2Cl2
PRO A **342573-48-2**

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 10 CASREACT COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 128:102040 CASREACT

TITLE: Functionalized ozonides by substitution reactions of chlorinated ozonides with difunctional alcohols

AUTHOR(S): Griesbaum, Karl; Quinkert, Ralf Olaf

CORPORATE SOURCE: Engler-Bunte-Institut, Bereich Petrochemie, Universitaet Karlsruhe, Karlsruhe, D-76128, Germany

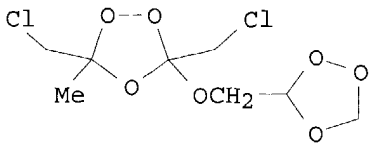
SOURCE: Liebigs Annalen/Recueil (1997), (12), 2581-2585
CODEN: LIARFV

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



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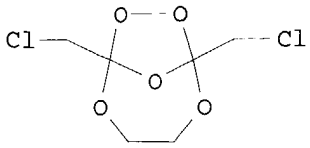
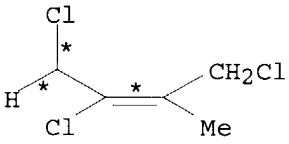


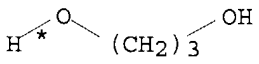
III

AB Substitution of 3-chloro-3,5-bis(chloromethyl)-5-methyl-1,2,4-trioxolane (I) with allyl alc. gave the corresponding diastereomeric allyloxy-substituted ozonides, which were converted into diozonides II by ozone treatment. Substitution of I with ethanediol or with 1,3-propanediol gave the corresponding hydroxyalkoxy-substituted ozonides, which were oxidized to the corresponding aldehydes. Reaction of 3,5-dichloro-3,5-bis(chloromethyl)-1,2,4-trioxolane with ethanediol gave the corresponding bis(hydroxy)-substituted ozonide as well as bicyclic ozonide III by reaction with ethanediol in a ratio of 1:1.

RX(10) OF 19 2 **A** + 2 **Z** ===> **AA** + X...

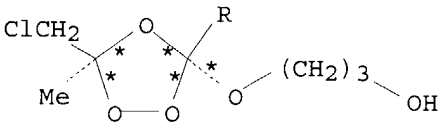


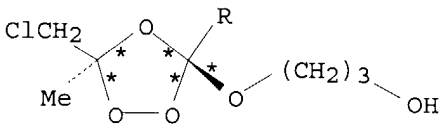
2 A

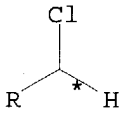


2 Z

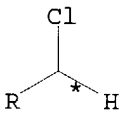
(10)







AA
YIELD 12%



X
YIELD 35%

RX(10) RCT A **73900-41-1**

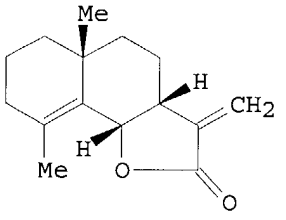
STAGE(1)
RGT E 10028-15-6 Ozone
SOL 109-66-0 Pentane

STAGE(2)
RCT Z **504-63-2**
RGT F 584-08-7 K2CO3

STAGE(3)

RGT M 7732-18-5 Water
PRO AA **201222-71-1**, X 201222-72-2

L3 ANSWER 3 OF 10 CASREACT COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 120:107377 CASREACT
TITLE: Synthesis of a stereoisomer of frullanolide utilizing the intramolecular cyclization of ω-formyl-2-alkenylsilane
AUTHOR(S): Kuroda, Chiaki; Shimizu, Shigeru; Haishima, Takahiro; Satoh, James Y.
CORPORATE SOURCE: Dep. Chem., Rikkyo Univ., Tokyo, 171, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1993), 66(8), 2298-303
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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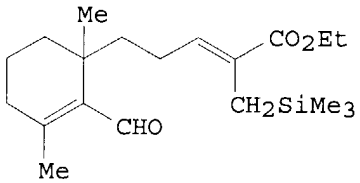

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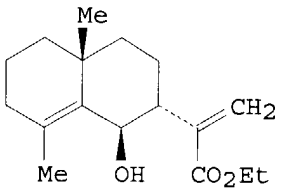
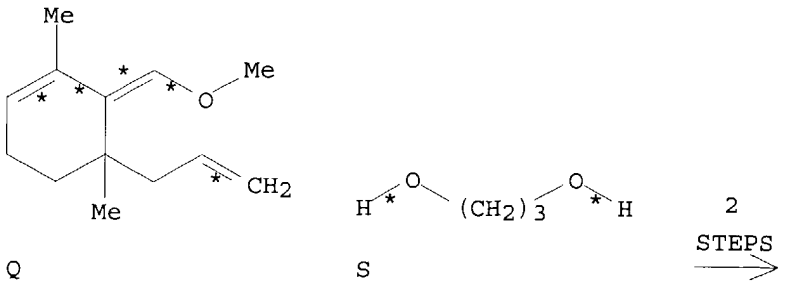


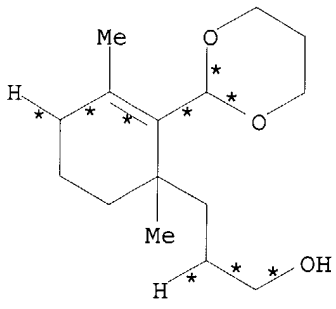
III

AB Synthesis of 10-epi-frullanolide (I) is reported via the intramol. cyclization of a ω-formyl-α-trimethylsilylmethyl-α,β-unsatd. ester. The cyclization precursor, Et (Z)-5-(2-formyl-1,3-dimethyl-2-cyclohexenyl)-2-trimethylsilylmethyl-2-pentenoate (II), was prepared from 2,6-dimethyl-2-cyclohexen-1-one through the dialdehyde monoacetal as the key intermediate. Cyclization of II with tetrabutylammonium fluoride produced the hydroxy ester III having C(6α)-H and C(7β)-H, which was hydrolyzed, then subjected to Fujisawa's lactonization to afford I.

RX(13) OF 55 COMPOSED OF RX(4), RX(5)
RX(13) Q + **S** ===> **Y**



Q S



Y
YIELD 96%

RX(4) RCT Q 152429-50-0

STAGE(1)
RGT U 7647-01-0 HCl
SOL 7732-18-5 Water, 109-99-9 THF

STAGE(2)
RCT S **504-63-2**
CAT 24057-28-1 Pyridinium tosylate
SOL 71-43-2 Benzene
PRO T 152429-52-2

RX(5) RCT T 152429-52-2

STAGE(1)
RGT Z 109-63-7 BF3-Et2O, AA 16940-66-2 NaBH4, AB **513-35-9** Me2C:CHMe
SOL 513-35-9 Me2C:CHMe

STAGE(2)
RGT AC 7722-84-1 H2O2, AD 1310-73-2 NaOH
SOL 7732-18-5 Water
PRO Y **152429-54-4**

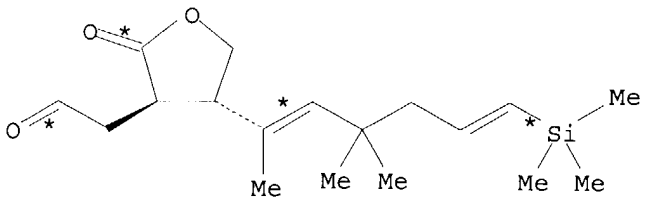
L3 ANSWER 4 OF 10 CASREACT COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 115:280316 CASREACT
TITLE: Synthesis of (+)-fragolide and (-)-pereniporin B via vinylsilane terminated cationic cyclization
AUTHOR(S): Burke, Steven D.; Shankaran, K.; Helber, Margaret Jones

CORPORATE SOURCE: Dep. Chem., Univ. Wisconsin, Madison, WI, 53706, USA
SOURCE: Tetrahedron Letters (1991), 32(36), 4655-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

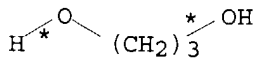
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Enantioselective syntheses of (+)-fragolide (I) and (-)-pereniporin B (II) are detailed. Marino's lactone annulation method, reaction of sulfone III and ZnCu/Cl3COCl to give lactone IV, was employed to establish relative and absolute stereochem. at carbon in the bicyclization substrate. Regio- and stereoselective oxidns. of tricyclic drimane precursors are described.

RX(35) OF 119 COMPOSED OF RX(5), RX(6), RX(7)
RX(35) 2 **P** + 2 **Q** ===> **V** + W

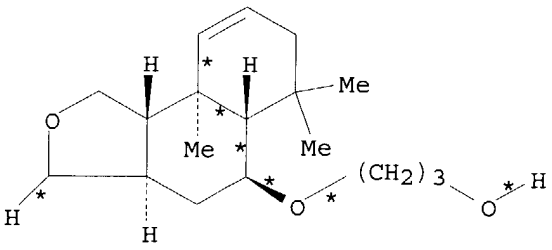


2 P

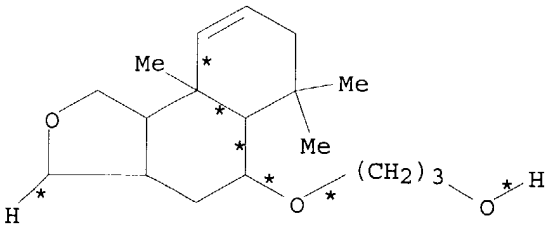


2 Q

3 STEPS



V



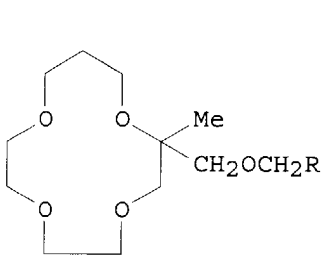
W

RX(5) RCT P **137266-31-0**, Q **504-63-2**
RGT S 77-78-1 Me2SO4
PRO R 137266-24-1
SOL 68-12-2 DMF
NTE 4Å zeolites

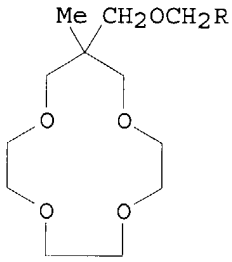
RX(6) RCT R 137266-24-1
PRO U 137266-25-2
NTE 2 steps

RX(7) RCT U 137266-25-2
RGT X 7550-45-0 TiCl4
PRO V **137266-26-3**, W 137331-24-9
SOL 75-09-2 CH2Cl2
NTE key step; 85% overall

L3 ANSWER 5 OF 10 CASREACT COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 114:42757 CASREACT
TITLE: Synthesis of methyl-substituted lariat ethers containing a 13-crown-4 ring
AUTHOR(S): Wakita, Ryuhei; Yonetani, Masayuki; Nakatsuji, Yohji; Okahara, Mitsuo
CORPORATE SOURCE: Fac. Eng., Osaka Univ., Osaka, 565, Japan
SOURCE: Journal of Heterocyclic Chemistry (1990), 27(5), 1337-9
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



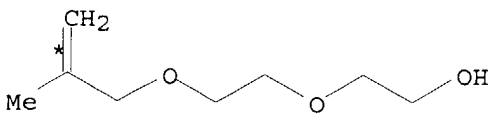
I



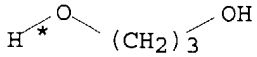
II

AB Convenient synthetic procedures for preparing two kinds of methyl-substituted lariat ethers containing a 13-crown-4-ring, I and II [R = CH2OMe, (CH2)8Me, 2-tetrahydrofuryl], are described. I were obtained from the reaction of 2-bromomethyl-2-methyl-13-crown-4 (III) with the appropriate alkoxide. III was prepared without the need for prior protection of the bromomethyl group. For the synthesis of II, which possess an electron-donating group on the central carbon of the tri-Me moiety of the 13-crown-4-ring, the substituents were introduced before cyclization.

RX(5) OF 9 **M** + **N** ===> **I**...

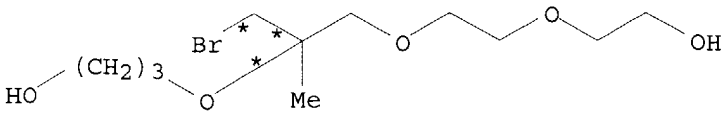


M



N

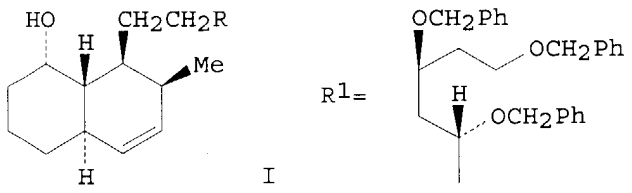
(5) →



I
YIELD 48%

RX(5) RCT M **121343-32-6**, N **504-63-2**
RGT L 128-08-5 Bromosuccinimide
PRO I **131526-53-9**
SOL 504-63-2 HO(CH2)3OH

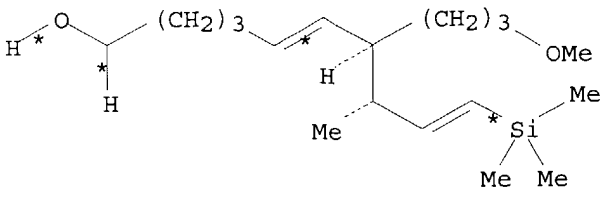
L3 ANSWER 6 OF 10 CASREACT COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 113:40247 CASREACT
TITLE: Synthesis of optically active mevinic acid subunits via acetal initiated/vinylsilane terminated polyene cyclizations
AUTHOR(S): Burke, Steven D.; Takeuchi, Kumiko; Murtiashaw, C. W.; Liang, D. W. M.
CORPORATE SOURCE: Dep. Chem., Univ. South Carolina, Columbia, SC, 29208, USA
SOURCE: Tetrahedron Letters (1989), 30(46), 6299-302
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

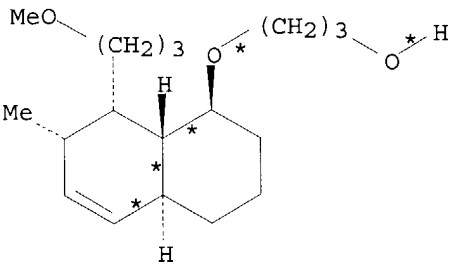
AB Efficient routes to optically active octahydronaphthalenol mevinic acid subunits I (R = CH2OMe, R1) via vinylsilane-mediated polyene cyclizations initiated by trimethylenedioxy acetals are detailed. Enantioselective alkynone redns. and Ireland-Claisen rearrangements serve to establish and transfer absolute stereochem.

RX(26) OF 100 COMPOSED OF RX(7), RX(8)
RX(26) 3 **AD** ===> **AL** + AM + AN

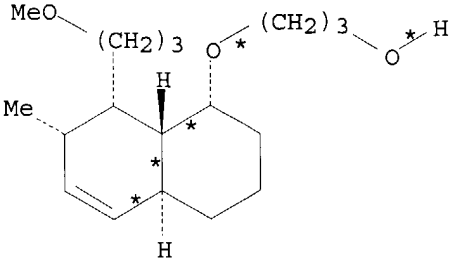


3 AD

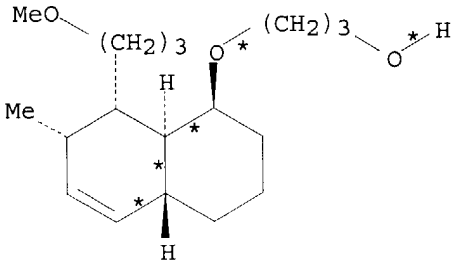
2 STEPS



AL
YIELD 91%(17)



AM
YIELD 91%(10)



AN
YIELD 91%(73)

RX(7) RCT AD **128061-45-0**

STAGE(1)
RGT W 79-37-8 (COCl)2, X 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

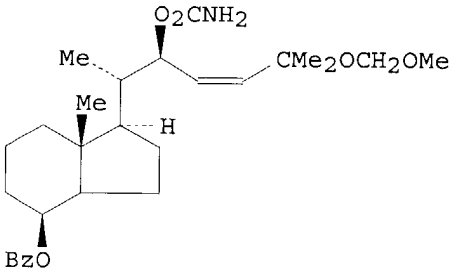
STAGE(2)
RGT Y 121-44-8 Et3N

STAGE(3)
RGT AI **504-63-2** HO(CH2)3OH
CAT 24057-28-1 Pyridinium tosylate
SOL 71-43-2 Benzene
PRO AH 128061-46-1

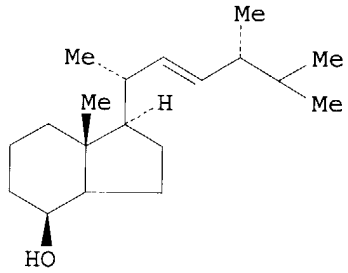
RX(8) RCT AH 128061-46-1

RGT AO 7550-45-0 TiCl4
PRO AL **128038-02-8**, AM 128038-03-9, AN 128038-04-0
SOL 75-09-2 CH2Cl2

L3 ANSWER 7 OF 10 CASREACT COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 109:73744 CASREACT
TITLE: Stereoselective synthesis of 25-hydroxyvitamin D2 side chain via the acetal template route
AUTHOR(S): Castedo, L.; Granja, J.; Maestro, M. A.; Mourino, A.
CORPORATE SOURCE: Dep. Quim. Org., Fac. Quim., Santiago de Compostela, Spain
SOURCE: Tetrahedron Letters (1987), 28(39), 4589-90
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



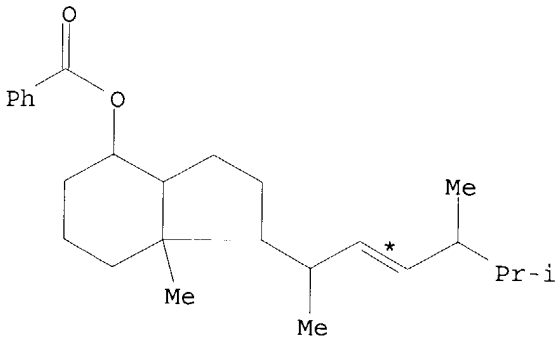
I



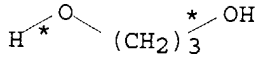
II

AB An improved synthesis of the vitamin intermediate I from II was described.

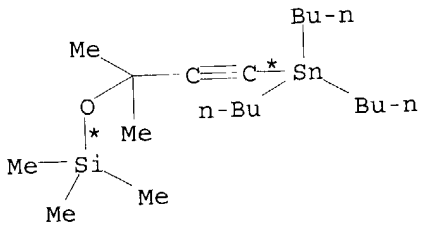
RX(31) OF 54 COMPOSED OF RX(2), RX(4), RX(8)
RX(31) 2 **C** + 2 **N** + 2 V ===> **W** + X



2 C

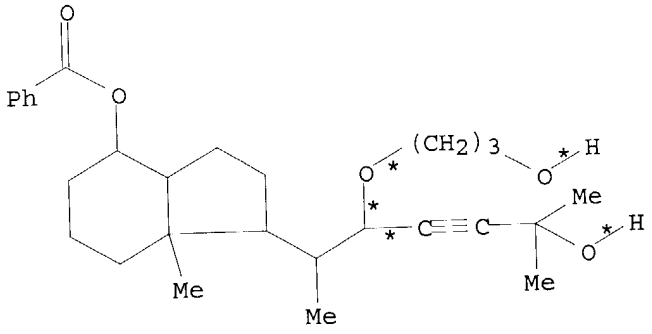


2 N

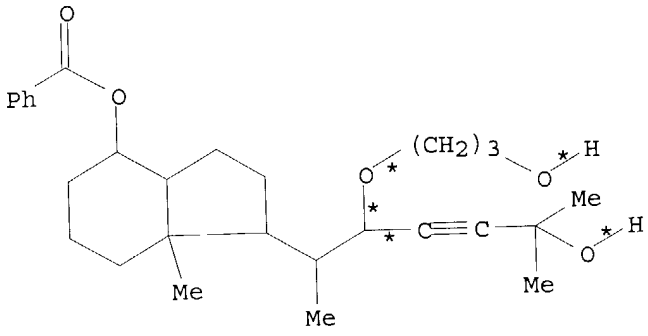


2 V

3
STEPS



W
YIELD 85%(67)



X
YIELD 85%(33)

RX(2) RCT C **68702-86-3**

STAGE(1)
RGT G 10028-15-6 Ozone, D 110-86-1 Pyridine
SOL 67-56-1 MeOH, 75-09-2 CH2Cl2

STAGE(2)
RGT H 122-52-1 P(OEt)3
SOL 67-56-1 MeOH, 75-09-2 CH2Cl2
PRO F 66774-71-8

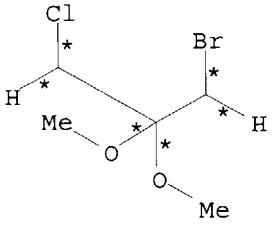
RX(4) RCT N **504-63-2**, F 66774-71-8
RGT P 109-63-7 BF3-Et2O
PRO O 115527-13-4
SOL 109-99-9 THF

RX(8) RCT V 115527-16-7, O 115527-13-4
RGT Y 7550-45-0 TiCl4
PRO W **115527-17-8**, X 115589-94-1
SOL 75-09-2 CH2Cl2

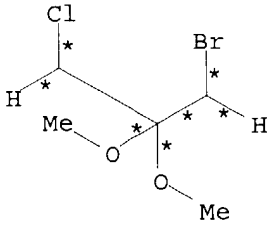
L3 ANSWER 8 OF 10 CASREACT COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 107:133679 CASREACT
TITLE: Thermal reactions of cyclopropenone ketals. Key mechanistic features and scope of the cycloaddition reactions of delocalized singlet vinylcarbenes: three-carbon 1,1-/1,3-dipoles
AUTHOR(S): Boger, Dale L.; Brotherton, Christine E.
CORPORATE SOURCE: Dep. Med. Chem., Univ. Kansas, Lawrence, KS, 66045-2500, USA
SOURCE: Journal of the American Chemical Society (1986), 108(21), 6695-713
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Full details of the key mechanistic features and the preparative scope of the thermal reactions of cyclopropenone ketals which proceed by the thermal generation and subsequent cycloaddn. reactions of π-delocalized singlet vinylcarbenes, 3-carbon 1,1-/1,3-dipoles lacking octet stabilization, are described and include ω2a participation in cheletropic [π2s + ω2a] nonlinear cycloaddns. with an observable endo effect suitable for a one-step, stereoselective construction of cis-cyclopropaneacetic acid esters, formal π2a participation in [π2s + π2a] cycloaddns. suitable for the preparation of functionalized cyclopentenes in which each of the 5 carbons of the newly formed 5-membered ring may bear functionality capable of addnl. transformation, and π2a participation in [π4s + π2s] cycloaddns. with selected dienes in direct [3 + 4] cycloaddns. suitable for the preparation of functionalized cycloheptadienes capable of further elaboration to tropones/tropolones. The complementary scope of the thermal reactions of cyclopropenone ketals is demonstrated with the preparation of the complete range of (methoxycarbonyl)tropones, 2-, 3-, and 4-(methoxycarbonyl)tropone and tropone, utilizing the appropriate choice of starting diene and complementary choice of conditions for promoting the thermal [3 + 4] or [4 + 2] cycloaddn. of a cyclopropenone ketal. Addnl. details of a preliminary study of the scope of the cycloaddn. reactions of the apparent π-delocalized singlet vinylcarbene with C-heteroatom double bonds are described.

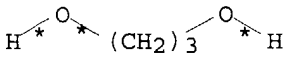
RX(91) OF 123 COMPOSED OF RX(51), RX(52), RX(6)
RX(91) 2 CO + 2 **CP** + 2 **N** ===> **O** + M



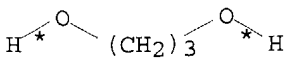
CO



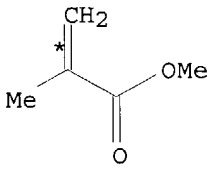
CO



CP

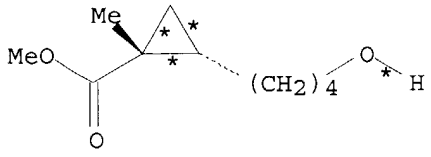


CP

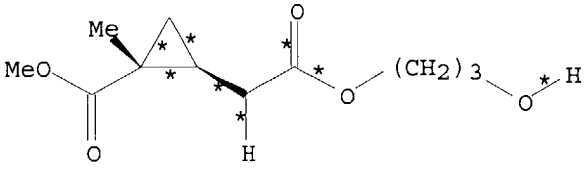


2 N

3 STEPS



O



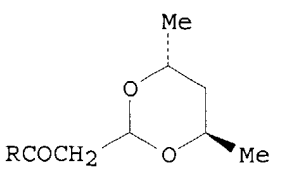
M

RX(51) RCT CO 22089-54-9, CP **504-63-2**
RGT CM 7664-93-9 H2SO4
PRO CQ 60935-30-0
SOL 7732-18-5 Water

RX(52) RCT CQ 60935-30-0
RGT CR 17242-52-3 KNH2
PRO A 60935-21-9
CAT 7705-08-0 FeCl3
SOL 7664-41-7 NH3, 60-29-7 Et2O

RX(6) RCT A 60935-21-9, N 80-62-6
PRO O **103384-75-4**, M 94923-06-5
SOL 71-43-2 Benzene

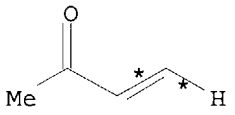
L3 ANSWER 9 OF 10 CASREACT COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 106:213861 CASREACT
TITLE: Palladium(II)-catalyzed acetalization of terminal olefins bearing electron-withdrawing substituents with optically active diols
AUTHOR(S): Hosokawa, Takahiro; Ohta, Toshiyuki; Kanayama, Satoshi; Murahashi, Shunichi
CORPORATE SOURCE: Fac. Eng. Sci., Osaka Univ., Osaka, 560, Japan
SOURCE: Journal of Organic Chemistry (1987), 52(9), 1758-64
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



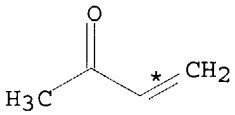
II

AB Terminal alkenes bearing electron-withdrawing substituents, such as CH2:CH2:CHCOR (R = Ph, Me, Me3C), CH2:CHCO2Me, and CH2:CHCN, are regioselectively acetalized at the terminal carbon by diols in the presence of PdCl2 and CuCl in MeOCH2CH2OMe at 50° under an atmospheric of O. The use of optically active (R,R)-2,4-pentanediol (I) gives homochiral cyclic acetals of aldehyde precursors, for example, II (R = Ph, Me, Me3C), in good yields. The reactivity of alkenes appears to decrease in the order: CH2:CHPh > CH2:CHCO2Me > CH2:CHCOR. Acetalization of CH2:CHCOR is accompanied by the formation of Michael-type adducts such as RCOCH2CH2OCHMeCH2CH(OH)Me. Their formation can be prevented by the use of Na2HPO4 as an additive. Although in an early stage of the reaction of CD2:CHPh with I, a statistical D scrambling of the starting alkene occurs, no such scrambling is observed with CD2:CHCOPh. Addnl., the acetalization of CD2:CHCOPh with I results in 1,2 deuterium migration, together with 25% D loss. These results are explained by reaction pathways involving oxypalladation, Pd-H elimination, and subsequent ring closure giving enol ether. A catalytic cycle involving the oxygenation of Pd-H species with mol. oxygen is proposed.

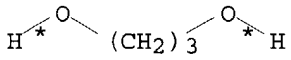
RX(9) OF 36 2 **J** + 2 **P** ===> S + **T**...



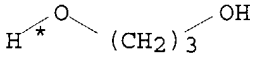
J



J

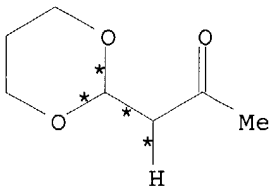


P

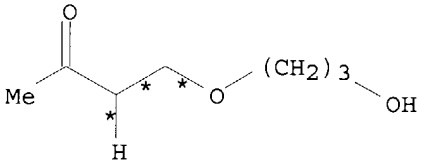


P

(9)



S
YIELD 45%



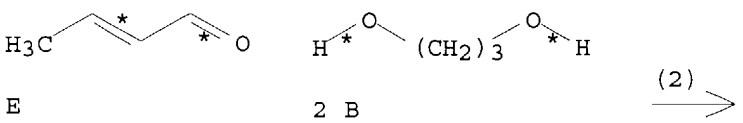
T
YIELD 8%

RX(9) RCT J **78-94-4**, P **504-63-2**
RGT E 7782-44-7 O2

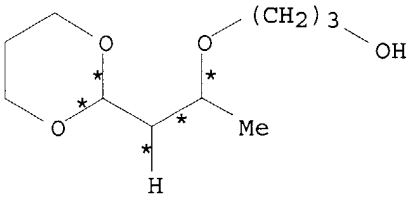
PRO S 55558-31-1, T **87971-38-8**
CAT 7647-10-1 PdCl2, 7758-89-6 CuCl
SOL 110-71-4 (CH2OMe)2

L3 ANSWER 10 OF 10 CASREACT COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 102:220779 CASREACT
TITLE: Acetals and ethers - XIII. Reaction products of 2-butenal with ethylene glycol
AUTHOR(S): Piasecki, Andrzej
CORPORATE SOURCE: Inst. Org. Polym. Technol., Techn. Univ. Wroclaw, Wroclaw, 50-370, Pol.
SOURCE: Tetrahedron (1984), 40(23), 4893-6
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The unsatd. cyclic acetal, 2-(1-propenyl)-1,3-dioxolane, was an intermediate in the 4-MeC6H4SO3H-catalyzed reaction of 2-butenal with excess ethylene glycol. The final product was 2-[2-(2-hydroxyethoxy)propyl]-1,3-dioxolane, and a small amount of cis- and trans-5-(2-hydroxyethoxy)-7-methyl-1,4-dioxepane.

RX(2) OF 8 **E** + 2 **B** ===> **F**



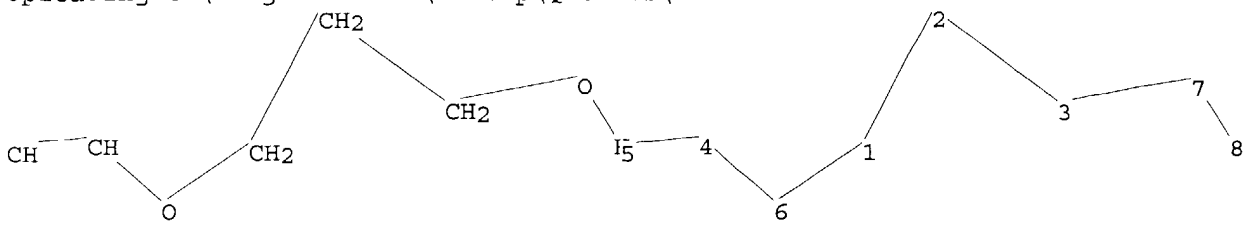
E 2 B



F

RX(2) RCT E **4170-30-3**, B **504-63-2**
PRO F **96424-48-5**
CAT 104-15-4 TsOH

>
Uploading C:\Program Files\Stnexp\Queries\679174.str

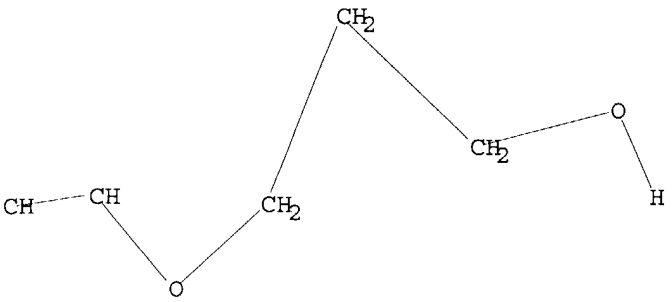


chain nodes :
1 2 3 4 5 6 7 8
chain bonds :
1-2 1-6 2-3 3-7 4-5 4-6 7-8
exact/norm bonds :
4-6
exact bonds :
1-2 1-6 2-3 3-7 4-5 7-8

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS

L4 STRUCTURE UPLOADED

=> d
L4 HAS NO ANSWERS
L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l4
SAMPLE SEARCH INITIATED 15:34:13 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 21528 TO ITERATE

4.6% PROCESSED 1000 ITERATIONS 5 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

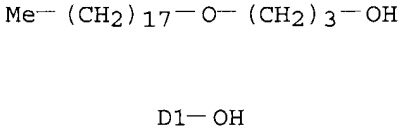
FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 421786 TO 439334
PROJECTED ANSWERS: 1530 TO 2774

L5 5 SEA SSS SAM L4

=> s his
L6 11725 HIS

=> d scan l5

L5 5 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN Propanediol, 3-(octadecyloxy)- (9CI)
MF C21 H44 O3
CI IDS

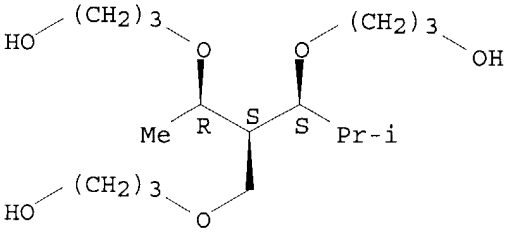


D1—OH

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L5 5 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 1-Propanol, 3,3'-[[2-[1-(3-hydroxypropoxy)ethyl]-1-(1-methylethyl)-1,3-propanediyl]bis(oxy)]bis-, [1S-[1R*,2R*(S*)]]- (9CI)
MF C17 H36 O6

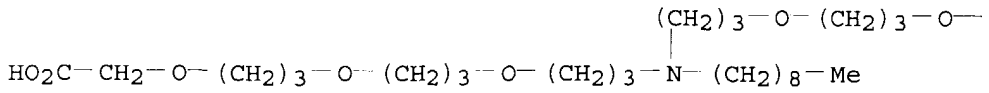
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

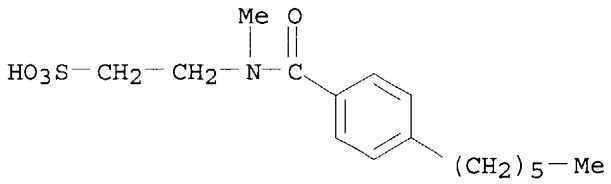
L5 5 ANSWERS REGISTRY COPYRIGHT 2004 ACS on STN
IN 3,7,11,19,23-Pentaoxa-15-azahexacosanoic acid, 26-hydroxy-15-nonyl-, sodium salt, compd. with N-p-hexylbenzoyl-N-methyltaurine (6CI)
MF C29 H59 N O8 . C16 H25 N O4 S . Na

CM 1

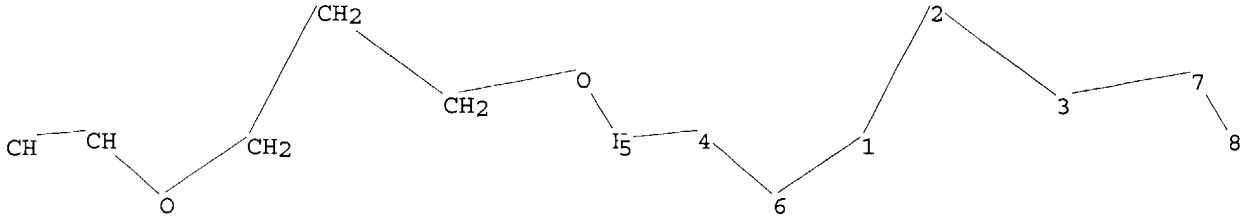


— $(CH_2)_3$ — OH

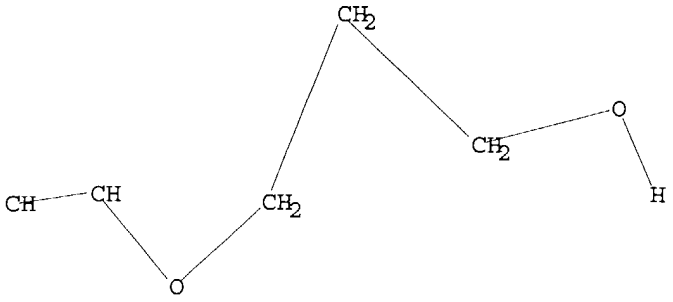
CM 2



```
**********************************************************************

=>
Uploading C:\Program Files\Stnexp\Queries\679174.str
```

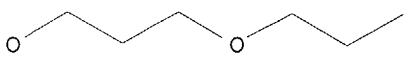



```
chain nodes :
1  2  3  4  5  6  7  8
chain bonds :
1-2  1-6  2-3  3-7  4-5  4-6  7-8
exact/norm bonds :
4-6
exact bonds :
1-2  1-6  2-3  3-7  4-5  7-8


Match level :
1:CLASS  2:CLASS  3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:CLASS  8:CLASS



L3       STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3                STR
```




```
Structure attributes must be viewed using STN Express query preparation.


=> s 2/o  not n/els
       1796054 2/O
       5757375 N/ELS
L4      617733 2/O  NOT N/ELS

=> s l4 not (s/els or x/els or m/els)
       1840876 S/ELS
             0 X/ELS
             0 M/ELS
L5      526528 L4 NOT (S/ELS OR X/ELS OR M/ELS)

=> s l5 not pms/ci
```

```
'CI' IS NOT A VALID FIELD CODE
             0 PMS/CI
L6       526528 L5 NOT PMS/CI

=> s l3 subset-l5
MISSING OPERATOR L3 SUBSET-L5
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> s l3 subset=l5
ENTER SUBSET SEARCH SCOPE - SAMPLE, FULL, RANGE, OR (END):full
FULL SUBSET SEARCH INITIATED 17:55:28 FILE 'BEILSTEIN'
FULL SUBSET SCREEN SEARCH COMPLETED -   3915 TO ITERATE

100.0% PROCESSED    3915 ITERATIONS                          46 ANSWERS
SEARCH TIME: 00.00.15

L7            46 SEA SUB=L5 SSS FUL L3

=> s l7 and 1-5/nr
'NR' IS NOT A VALID FIELD CODE
             0 1-5/NR
L8           0 L7 AND 1-5/NR

=> s l7 and pheny?
       2387182 PHENY?
L9           8 L7 AND PHENY?

=> s l7 not l9
L10         38 L7 NOT L9

=> d ide 38


L10  ANSWER 38 OF 38 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

     Beilstein Records (BRN):        1697426
     Beilstein Pref. RN (BPR):       4161-22-2
     CAS Reg. No. (RN):              4161-22-2
     Chemical Name (CN):             3-propoxy-propan-1-ol, trimethylene
                                     glycol-monopropyl ether
     Autonom Name (AUN):             3-propoxy-propan-1-ol
     Molec. Formula (MF):            C6 H14 O2
     Molecular Weight (MW):          118.18
     Lawson Number (LN):             523, 307
     Compound Type (CTYPE):          acyclic
     Constitution ID (CONSID):       1486956
     Tautomer ID (TAUTID):           1545775
     Beilstein Citation (BSO):       1-01-00-00247, 4-01-00-02495, 5-01, 6-01
     Entry Date (DED):               1989/02/27
     Update Date (DUPD):             2000/02/29
```




```
  Field Availability:

    Code      Name                                      Occurrence
    ==========================================================
```

BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	2
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	4
ED	Entry Date	1
UPD	Update Date	1
BP	Boiling Point	7
CDER	Chemical Derivative	1
DEN	Density (Liquid)	2
FINFO	Further Information	1
LIQPH	Liquid Phase	1
MECM	Mechanical & Physical Property (MCS)	1
NMR	Nuclear Magnetic Resonance	1
RI	Refractive Index	3
SOUND	Acoustic Property	3

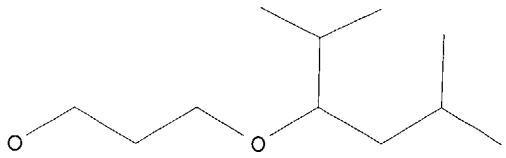
This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	9
RXREA	Substance is Reaction Reactant	3
RXPRO	Substance is Reaction Product	6

```
=> s l10 and (isopro? or methylethyl or tertiary butyl )
        276143 ISOPRO?
          9515 METHYLETHYL
            43 TERTIARY
        561238 BUTYL
             7 TERTIARY BUTYL
                 (TERTIARY(W)BUTYL)
L11          2 L10 AND (ISOPRO? OR METHYLETHYL OR TERTIARY BUTYL )

=> d ide 1-2
```

L11 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	6716050
Chemical Name (CN):	**3-(1-isopropyl-3-methyl-butoxy)-propan-1-ol**
Autonom Name (AUN):	**3-(1-isopropyl-3-methyl-butoxy)-propan-1-ol**
Molec. Formula (MF):	C11 H24 O2
Molecular Weight (MW):	188.31
Lawson Number (LN):	523, 347
Compound Type (CTYPE):	acyclic
Constitution ID (CONSID):	5799856
Tautomer ID (TAUTID):	6354447
Beilstein Citation (BSO):	6-01
Entry Date (DED):	1994/07/18
Update Date (DUPD):	1994/07/18



Field Availability:

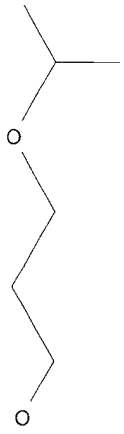
Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
FS	File Segment	1
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
DEN	Density (Liquid)	1
NMR	Nuclear Magnetic Resonance	1
RI	Refractive Index	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

L11 ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	1732698
Beilstein Pref. RN (BPR):	110-48-5
CAS Reg. No. (RN):	110-48-5
Chemical Name (CN):	**3-isopropoxy-propan-1-ol**
Autonom Name (AUN):	**3-isopropoxy-propan-1-ol**
Molec. Formula (MF):	C6 H14 O2
Molecular Weight (MW):	118.18
Lawson Number (LN):	523, 308
Compound Type (CTYPE):	acyclic
Constitution ID (CONSID):	1568042
Tautomer ID (TAUTID):	1643021
Beilstein Citation (BSO):	4-01-00-02495, 5-01
Entry Date (DED):	1989/02/27
Update Date (DUPD):	1997/12/03



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	2
ED	Entry Date	1
UPD	Update Date	1
BP	Boiling Point	3
CDER	Chemical Derivative	1
RI	Refractive Index	2
XREF	Crossfile Reference	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	2

=> d frxpro 1

L11 ANSWER 1 OF 2 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:
RX

Reaction ID (.ID):	1754057
Reactant BRN (.RBRN):	1340707, 3535134
Reactant (.RCT):	2-isopropyl-<1,3>dioxane, isobutylmagnesium bromide
Product BRN (.PBRN):	6716050
Product (.PRO):	3-(1-isopropyl-3-methyl-butoxy)-propan-1-

```
                                    ol
     No. of React. Details (.NVAR):  1

Reaction Details:
RX
     Reaction RID (.RID):           1754057.1
     Reaction Classification (.CL): Preparation
     Yield (.YDT):                  80 percent (BRN=6716050)
     Solvent (.SOL):                diethyl ether
     Time (.TIM):                   15 min
     Other Conditions (.COND):      Heating
     Reference(s):
     1. Mel'nitskii, I. A.; Glukhova, O. F.; Kiladze, T. K.; Kantor, E. A.;
        Rakhmankulov, D. L.; Paushkin, Ya. M., Dokl.Chem.(Engl.Transl.), CODEN:
        DKCHAY, 292, <1987>, 83-84, Dokl.Akad.Nauk SSSR Ser.Khim., CODEN:
        DASKAJ, 292(6), <1987>, 1390-1392; BABS-5868508


=> d frxpro 2


L11  ANSWER 2 OF 2 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:
RX
     Reaction ID (.ID):             6949345
     Product BRN (.PBRN):           1732698
     Product (.PRO):                3-isopropoxy-propan-1-ol
     No. of React. Details (.NVAR): 1

Reaction Details:
RX
     Reaction RID (.RID):           6949345.1
     Reaction Classification (.CL): Preparation (half reaction)
     Reference(s):
     1. Smith; Williams, J.Amer.Chem.Soc., CODEN: JACSAT, 91, <1969>, 5254,5259

Reaction:
RX
     Reaction ID (.ID):             3366
     Reactant BRN (.RBRN):          102382, 635639
     Reactant (.RCT):               oxetane, propan-2-ol
     Product BRN (.PBRN):           1732698
     Product (.PRO):                3-isopropoxy-propan-1-ol
     No. of React. Details (.NVAR): 1

Reaction Details:
RX
     Reaction RID (.RID):           3366.1
     Reaction Classification (.CL): Preparation
     Other Conditions (.COND):      1731204
     Note(s) (.COM):                Handbook
     Reference(s):
     1. Searles; Butler, J.Amer.Chem.Soc., CODEN: JACSAT, 76, <1954>, 56


=> d his

     (FILE 'HOME' ENTERED AT 17:48:46 ON 15 APR 2004)

     FILE 'REGISTRY' ENTERED AT 17:48:53 ON 15 APR 2004
L1         54830 S 3-PROPANEDIOL
L2            10 S 3-PROPANEDIOL AND C3H8O2/MF
```

UPD	Update Date	1
BP	Boiling Point	1
IR	Infrared Spectrum	1
PHARM	Pharmacological Data	1
RI	Refractive Index	2
XREF	Crossfile Reference	1

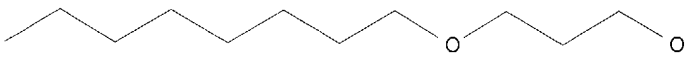
This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	2

=> d ide l12 12

L12 ANSWER 12 OF 36 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	6185575
Chemical Name (CN):	3-octyloxypropan-1-ol
Autonom Name (AUN):	3-octyloxy-propan-1-ol
Molec. Formula (MF):	C11 H24 O2
Molecular Weight (MW):	188.31
Lawson Number (LN):	523, 344
Compound Type (CTYPE):	acyclic
Constitution ID (CONSID):	5335889
Tautomer ID (TAUTID):	5806321
Beilstein Citation (BSO):	6-01
Entry Date (DED):	1993/10/20
Update Date (DUPD):	1995/05/11



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	1
NMR	Nuclear Magnetic Resonance	3

This substance also occurs in Reaction Documents:

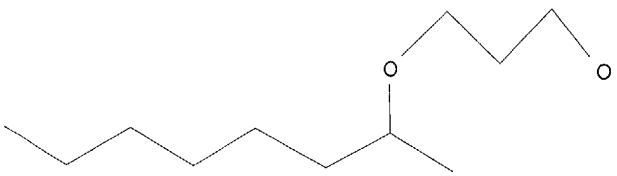
Code	Name	Occurrence

RX	Reaction Documents	2
RXPRO	Substance is Reaction Product	2

```
=> s l12 and methyl?
      2664228 METHYL?
L14           7 L12 AND METHYL?

=> d ide 7
```

L14 ANSWER 7 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	4304771
Chemical Name (CN):	**3-(1-methyl-heptyloxy)-propan-1-ol**
Autonom Name (AUN):	**3-(1-methyl-heptyloxy)-propan-1-ol**
Molec. Formula (MF):	C11 H24 O2
Molecular Weight (MW):	188.31
Lawson Number (LN):	523, 345
Compound Type (CTYPE):	acyclic
Constitution ID (CONSID):	3888340
Tautomer ID (TAUTID):	4144953
Beilstein Citation (BSO):	6-01
Entry Date (DED):	1992/07/20
Update Date (DUPD):	1992/09/22



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d frxpro 7

L14 ANSWER 7 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:
RX

Reaction ID (.ID):	1537307
Reactant BRN (.RBRN):	106557
Reactant (.RCT):	2-hexyl-2-methyl-<1,3>dioxane
Product BRN (.PBRN):	4304771
Product (.PRO):	3-(1-methyl-heptyloxy)-propan-1-ol
No. of React. Details (.NVAR):	1

Reaction Details:
RX

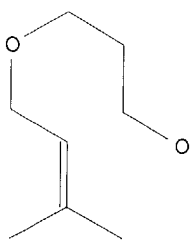
Reaction RID (.RID):	1537307.1
Reaction Classification (.CL):	Preparation
Yield (.YDT):	53 percent (BRN=4304771)
Reagent (.RGT):	trimethylsilyl trifluoromethanesulphonate (TMSOTf), BH3S*Me2
Solvent (.SOL):	CH2Cl2
Temperature (.T):	-78 Cel

Reference(s):
1. Hunter, Roger; Bartels, Birgit; Michael, Joseph P., Tetrahedron Lett., CODEN: TELEAY, 32(8), <1991>, 1095-1098; BABS-5539910

=> d 6

L14 ANSWER 6 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	5917293
Beilstein Pref. RN (BPR):	126274-83-7
CAS Reg. No. (RN):	126274-83-7
Chemical Name (CN):	**7-methyl-4-oxa-6-octen-1-ol**
Autonom Name (AUN):	**3-(3-methyl-but-2-enyloxy)-propan-1-ol**
Molec. Formula (MF):	C8 H16 O2
Molecular Weight (MW):	144.21
Lawson Number (LN):	523, 422
Compound Type (CTYPE):	acyclic
Constitution ID (CONSID):	5162765
Tautomer ID (TAUTID):	5614415
Beilstein Citation (BSO):	6-01
Entry Date (DED):	1993/07/22
Update Date (DUPD):	1997/08/11



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
IR	Infrared Spectrum	2
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	4

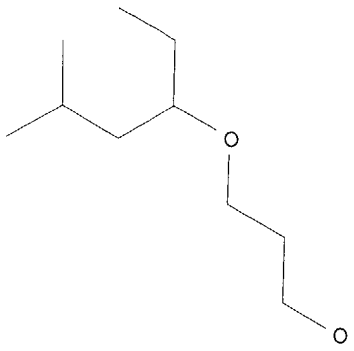
This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

=> d 5

L14 ANSWER 5 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN): 6185309
Chemical Name (CN): **3-(1-ethyl-3-methyl-butoxy)-propan-1-ol**
Autonom Name (AUN): **3-(1-ethyl-3-methyl-butoxy)-propan-1-ol**
Molec. Formula (MF): C10 H22 O2
Molecular Weight (MW): 174.28
Lawson Number (LN): 523, 337
Compound Type (CTYPE): acyclic
Constitution ID (CONSID): 5324570
Tautomer ID (TAUTID): 5800315
Beilstein Citation (BSO): 6-01
Entry Date (DED): 1993/10/20
Update Date (DUPD): 1994/10/31



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
BP	Boiling Point	2
IR	Infrared Spectrum	1
NMR	Nuclear Magnetic Resonance	3
RI	Refractive Index	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	3
RXPRO	Substance is Reaction Product	3

=> d frxpro 5

L14 ANSWER 5 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:
RX

Reaction ID (.ID):	1513740
Reactant BRN (.RBRN):	103967
Reactant (.RCT):	2-isobutyl-<1,3>dioxane
Product BRN (.PBRN):	6185309, 6715910
Product (.PRO):	3-(1-ethyl-3-methyl-butoxy)-propan-1-ol, 3-(3-methyl-butoxy)-propan-1-ol
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	1513740.1
Reaction Classification (.CL):	Preparation

Yield (.YDT): 0.02 mol (BRN=6185309), 0.02 mol (BRN=6715910)
Reagent (.RGT): diethylaluminum hydride, triethylaluminum
Solvent (.SOL): kerosene, hexane
Time (.TIM): 15 hour(s)
Other Conditions (.COND): Heating
Reference(s):
1. Volkov, A. A.; Kravets, E. Kh.; Zlot-skii, S. S.; Rakhmankulov, D. L., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 58, <1985>, 1419-1423, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 58(7), <1985>, 1547-1552; BABS-5880479

Reaction:
RX
Reaction ID (.ID): 1513739
Reactant BRN (.RBRN): 103967, 3587229
Reactant (.RCT): 2-isobutyl-<1,3>dioxane, triethylaluminium
Product BRN (.PBRN): 6715910, 6185309
Product (.PRO): 3-(3-methyl-butoxy)-propan-1-ol, 3-(1-ethyl-3-methyl-butoxy)-propan-1-ol
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 1513739.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 0.01 mol (BRN=6715910), 0.035 mol (BRN=6185309)
Reagent (.RGT): diethylaluminum hydride
Solvent (.SOL): kerosene, hexane
Time (.TIM): 30 hour(s)
Other Conditions (.COND): Heating
Reference(s):
1. Volkov, A. A.; Kravets, E. Kh.; Zlot-skii, S. S.; Rakhmankulov, D. L., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 58, <1985>, 1419-1423, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 58(7), <1985>, 1547-1552; BABS-5880479

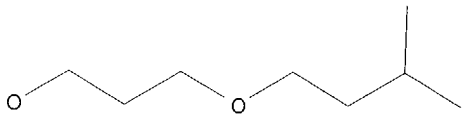
Reaction:
RX
Reaction ID (.ID): 1513738
Reactant BRN (.RBRN): 103967, 3587229
Reactant (.RCT): 2-isobutyl-<1,3>dioxane, triethylaluminium
Product BRN (.PBRN): 6185309
Product (.PRO): 3-(1-ethyl-3-methyl-butoxy)-propan-1-ol
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 1513738.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 68 percent (BRN=6185309)
Solvent (.SOL): hexane
Time (.TIM): 5 min
Temperature (.T): 70 Cel
Reference(s):
1. Volkov, A. A.; Zlotskii, S. S.; Kravets, E. Kh; Rakhmankulov, D. L., Dokl.Chem.(Engl.Transl.), CODEN: DKCHAY, 283, <1985>, 246-248, Dokl.Akad.Nauk SSSR Ser.Khim., CODEN: DASKAJ, 283(5), <1985>, 1194-1196; BABS-5773191

=> d 4

L14 ANSWER 4 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	6715910
Chemical Name (CN):	**3-(3-methyl-butoxy)-propan-1-ol**
Autonom Name (AUN):	**3-(3-methyl-butoxy)-propan-1-ol**
Molec. Formula (MF):	C8 H18 O2
Molecular Weight (MW):	146.23
Lawson Number (LN):	523, 326
Compound Type (CTYPE):	acyclic
Constitution ID (CONSID):	5798151
Tautomer ID (TAUTID):	6353156
Beilstein Citation (BSO):	6-01
Entry Date (DED):	1994/07/18
Update Date (DUPD):	1998/11/09



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
BP	Boiling Point	1
DEN	Density (Liquid)	1
IR	Infrared Spectrum	1
NMR	Nuclear Magnetic Resonance	2
RI	Refractive Index	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	4
RXPRO	Substance is Reaction Product	4

=> d frxpro 4

L14 ANSWER 4 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:
RX

Reaction ID (.ID):	4855860

Reactant BRN (.RBRN): 3535405, 102532
Reactant (.RCT): isobutylmagnesium bromide, <1,3>dioxane
Product BRN (.PBRN): 6715910
Product (.PRO): 3-(3-methyl-butoxy)-propan-1-ol
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 4855860.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 40 percent (BRN=6715910)
Reagent (.RGT): ZnBr2
Solvent (.SOL): diethyl ether
Time (.TIM): 2 hour(s)
Other Conditions (.COND): Heating
Reference(s):
1. Sunagatov, M. F.; Mel'nitskii, L. A.; Kantor, E. A., Russ.J.Gen.Chem., CODEN: RJGCEK, 67(2), <1997>, 270-272, Zh.Obshch.Khim., CODEN: ZOKHA4, 67(2), <1997>, 288-290; BABS-6089219

Reaction:
RX
Reaction ID (.ID): 1513740
Reactant BRN (.RBRN): 103967
Reactant (.RCT): 2-isobutyl-<1,3>dioxane
Product BRN (.PBRN): 6185309, 6715910
Product (.PRO): 3-(1-ethyl-3-methyl-butoxy)-propan-1-ol, 3-(3-methyl-butoxy)-propan-1-ol
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 1513740.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 0.02 mol (BRN=6185309), 0.02 mol (BRN=6715910)
Reagent (.RGT): diethylaluminum hydride, triethylaluminum
Solvent (.SOL): kerosene, hexane
Time (.TIM): 15 hour(s)
Other Conditions (.COND): Heating
Reference(s):
1. Volkov, A. A.; Kravets, E. Kh.; Zlot-skii, S. S.; Rakhmankulov, D. L., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 58, <1985>, 1419-1423, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 58(7), <1985>, 1547-1552; BABS-5880479

Reaction:
RX
Reaction ID (.ID): 1513739
Reactant BRN (.RBRN): 103967, 3587229
Reactant (.RCT): 2-isobutyl-<1,3>dioxane, triethylaluminium
Product BRN (.PBRN): 6715910, 6185309
Product (.PRO): 3-(3-methyl-butoxy)-propan-1-ol, 3-(1-ethyl-3-methyl-butoxy)-propan-1-ol
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 1513739.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 0.01 mol (BRN=6715910), 0.035 mol (BRN=6185309)
Reagent (.RGT): diethylaluminum hydride
Solvent (.SOL): kerosene, hexane

Time (.TIM): 30 hour(s)
Other Conditions (.COND): Heating
Reference(s):
1. Volkov, A. A.; Kravets, E. Kh.; Zlot-skii, S. S.; Rakhmankulov, D. L., J.Appl.Chem.USSR (Engl.Transl.), CODEN: JAPUAW, 58, <1985>, 1419-1423, Zh.Prikl.Khim.(Leningrad), CODEN: ZPKHAB, 58(7), <1985>, 1547-1552; BABS-5880479

Reaction:
RX
Reaction ID (.ID): 1488274
Reactant BRN (.RBRN): 102532, 3535134
Reactant (.RCT): <1,3>dioxane, isobutylmagnesium bromide
Product BRN (.PBRN): 6715910
Product (.PRO): 3-(3-methyl-butoxy)-propan-1-ol
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 1488274.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 73 percent (BRN=6715910)
Solvent (.SOL): diethyl ether
Time (.TIM): 15 min
Other Conditions (.COND): Heating
Reference(s):
1. Mel'nitskii, I. A.; Glukhova, O. F.; Kiladze, T. K.; Kantor, E. A.; Rakhmankulov, D. L.; Paushkin, Ya. M., Dokl.Chem.(Engl.Transl.), CODEN: DKCHAY, 292, <1987>, 83-84, Dokl.Akad.Nauk SSSR Ser.Khim., CODEN: DASKAJ, 292(6), <1987>, 1390-1392; BABS-5868508

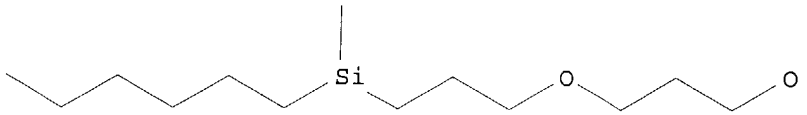
=> d frxpro 3 ide

L14 ANSWER 3 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:
RX
Reaction ID (.ID): 3662167
Reactant BRN (.RBRN): 6720068
Reactant (.RCT): 3-<3-(hexyl-methyl-silanyl)-propoxy>-propionic acid methyl ester
Product BRN (.PBRN): 6716507
Product (.PRO): 3-<3-(hexylmethylsilyl)propoxy>-1-propanol
No. of React. Details (.NVAR): 1

Reaction Details:
RX
Reaction RID (.RID): 3662167.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 72 percent (BRN=6716507)
Reagent (.RGT): LiAlH4
Solvent (.SOL): diethyl ether
Time (.TIM): 10 hour(s)
Temperature (.T): 20 Cel
Reference(s):
1. Sultanov, R. A.; Gazarov, T. Sh.; Saryev, G. A., J.Gen.Chem.USSR (Engl.Transl.), CODEN: JGCHA4, 54, <1984>, 1005-1007, Zh.Obshch.Khim., CODEN: ZOKHA4, 54(5), <1984>, 1122-1125; BABS-5871217
Beilstein Records (BRN): 6716507
Chemical Name (CN): 3-<3-(hexylmethylsilyl)propoxy>-1-propanol
Autonom Name (AUN): **3-<3-(hexyl-methyl-silanyl)-propoxy>-propan-1-ol**

Molec. Formula (MF):	C13 H30 O2 Si
Molecular Weight (MW):	246.46
Lawson Number (LN):	3803, 3798, 3777, 523
Compound Type (CTYPE):	acyclic
Constitution ID (CONSID):	5818489
Tautomer ID (TAUTID):	6367435
Beilstein Citation (BSO):	6-04
Entry Date (DED):	1994/07/18
Update Date (DUPD):	1994/07/19



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	4
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1
BP	Boiling Point	1
DEN	Density (Liquid)	1
IR	Infrared Spectrum	1
RI	Refractive Index	1

This substance also occurs in Reaction Documents:

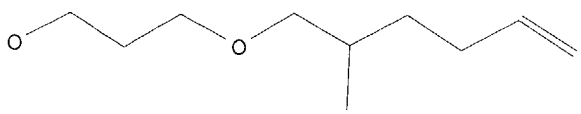
Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d ide 2

L14 ANSWER 2 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	7914336
Chemical Name (CN):	**3-(2-methyl-hex-5-enyloxy)-propan-1-ol**
Autonom Name (AUN):	**3-(2-methyl-hex-5-enyloxy)-propan-1-ol**
Molec. Formula (MF):	C10 H20 O2
Molecular Weight (MW):	172.27
Lawson Number (LN):	523, 432
Compound Type (CTYPE):	acyclic
Constitution ID (CONSID):	6749116

Tautomer ID (TAUTID): 7484361
Beilstein Citation (BSO): 6-01
Entry Date (DED): 1998/11/09
Update Date (DUPD): 1998/11/09



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

=> d frxpro 2

L14 ANSWER 2 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:
RX
Reaction ID (.ID): 4870816
Reactant BRN (.RBRN): 3587197, 2071854
Reactant (.RCT): trimethylaluminium, 3-allyloxy-propan-1-ol
Product BRN (.PBRN): 969155, 7914336
Product (.PRO): propane-1,3-diol, 3-(2-methyl-hex-5-enyloxy)-propan-1-ol
No. of React. Details (.NVAR): 1

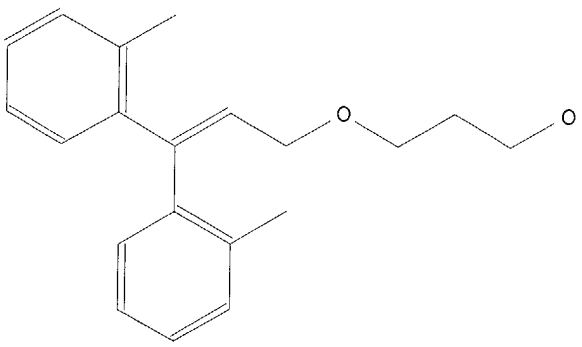
Reaction Details:
RX
Reaction RID (.RID): 4870816.1
Reaction Classification (.CL): Preparation
Yield (.YDT): 27 percent (BRN=7914336)
Catalyst (.CAT): (dppp)NiCl2
Solvent (.SOL): toluene
Reference(s):
1. Taniguchi, Takahiko; Ogasawara, Kunio, Chem.Commun., CODEN: CHCOFS(15),

<1998>, 1531-1532; BABS-6094785

=> d ide 1

L14 ANSWER 1 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Beilstein Records (BRN):	8496244
Chemical Name (CN):	**3-((-bis(2-methylphenyl)-1-propen-3-yl)oxy)-1-propanol**
Autonom Name (AUN):	3-(3,3-di-o-tolyl-allyloxy)-propan-1-ol
Molec. Formula (MF):	C20 H24 O2
Molecular Weight (MW):	296.41
Lawson Number (LN):	5590, 523
Compound Type (CTYPE):	isocyclic
Constitution ID (CONSID):	7203783
Tautomer ID (TAUTID):	7990827
Entry Date (DED):	2000/07/18
Update Date (DUPD):	2000/07/18



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
ED	Entry Date	1
UPD	Update Date	1
NMR	Nuclear Magnetic Resonance	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

=> d frxpro

L14 ANSWER 1 OF 7 BEILSTEIN COPYRIGHT 2004 BEILSTEIN MDL on STN

Reaction:
RX

Reaction ID (.ID):	8536350
Reactant BRN (.RBRN):	969155, 8486168
Reactant (.RCT):	propane-1,3-diol, 3-bromo-1,1-bis(2-methylphenyl)-1-propene
Product BRN (.PBRN):	8496244
Product (.PRO):	3-(3,3-di-o-tolyl-allyloxy)-propan-1-ol
No. of React. Details (.NVAR):	1

Reaction Details:
RX

Reaction RID (.RID):	8536350.1
Reaction Classification (.CL):	Multistage
Yield (.YDT):	31 percent (BRN=8496244)
Nr. of Stages (.SNR):	2
Stage 1	
Reagent (.RGT):	nBuLi
Solvent (.SOL):	hexane
Time (.TIM):	0.5 hour(s)
Temperature (.T):	20 Cel
Reaction Type (.TYP):	Metallation
Stage 2	
Stage reactant (.SRCT):	3-bromo-1,1-bis(2-methylphenyl)-1-propene
Stage Reactant BRN (.SRBRN):	8486168
Solvent (.SOL):	hexane
Time (.TIM):	36 hour(s)
Temperature (.T):	75 Cel
Reaction Type (.TYP):	Etherification

Reference(s):

1. Andersen, Knud Erik; Soerensen, Jan L.; Huusfeldt, Per O.; Knutsen, Lars J. S.; Lau, Jesper; Lundt, Behrend F.; Petersen, Hans; Suzdak, Peter D.; Swedberg, Michael D. B., J.Med.Chem., CODEN: JMCMAR, 42(21), <1999>, 4281 - 4291; BABS-6228258

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